



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:58 AM UTC

PDB ID : 4DX9 / pdb_00004dx9
Title : ICAP1 in complex with integrin beta 1 cytoplasmic tail
Authors : Liu, W.; Draheim, K.; Zhang, R.; Calderwood, D.A.; Boggon, T.J.
Deposited on : 2012-02-27
Resolution : 2.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

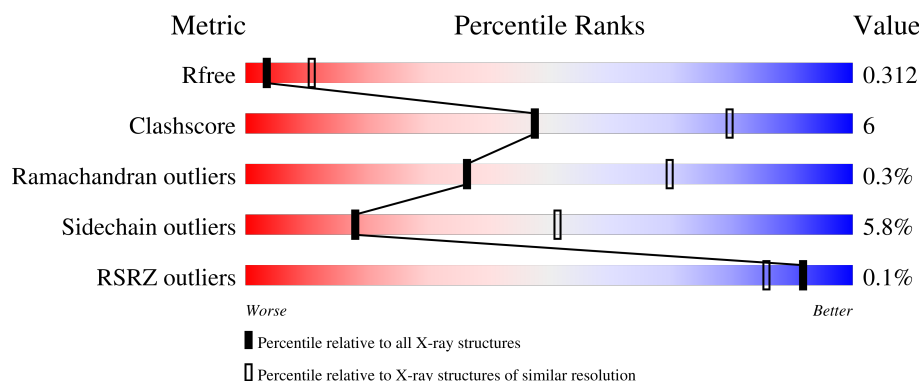
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	157	 61% 9% 30%
1	1	157	 61% 14% 25%
1	2	157	 55% 42%
1	3	157	 57% 8% 34%
1	4	157	 61% 19% 18%

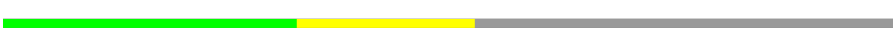
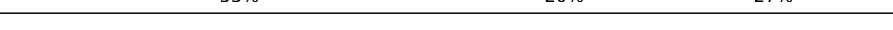
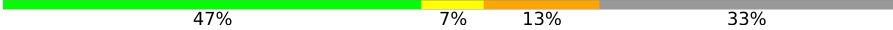
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Mol	Chain	Length	Quality of chain
1	5	157	
1	A	157	
1	C	157	
1	E	157	
1	G	157	
1	I	157	
1	K	157	
1	M	157	
1	O	157	
1	Q	157	
1	S	157	
1	U	157	
1	W	157	
1	Y	157	
1	a	157	
1	c	157	
1	e	157	
1	g	157	
1	i	157	
1	k	157	
1	m	157	
1	o	157	
1	q	157	
1	s	157	
1	u	157	

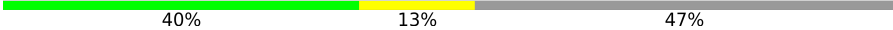
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Mol	Chain	Length	Quality of chain
1	w	157	
1	y	157	
2	6	15	
2	7	15	
2	8	15	
2	9	15	
2	B	15	
2	D	15	
2	F	15	
2	H	15	
2	J	15	
2	L	15	
2	N	15	
2	P	15	
2	R	15	
2	T	15	
2	V	15	
2	X	15	
2	Z	15	
2	b	15	
2	d	15	
2	f	15	
2	h	15	
2	j	15	
2	l	15	

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Mol	Chain	Length	Quality of chain
2	n	15	 73%27%
2	p	15	 20%13%67%
2	r	15	 13%87%
2	t	15	 40%13%47%
2	v	15	 33%20%47%
2	x	15	 13%13%73%
2	z	15	 33%67%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29306 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Integrin beta-1-binding protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	Se	0	0	0
			844	547	134	157	4	2			
1	0	110	Total	C	N	O	S	Se	0	0	0
			858	558	138	156	4	2			
1	k	105	Total	C	N	O	S	Se	0	0	0
			827	535	133	153	4	2			
1	m	127	Total	C	N	O	S	Se	0	0	0
			991	635	158	192	4	2			
1	1	118	Total	C	N	O	S	Se	0	0	0
			919	591	147	175	4	2			
1	C	127	Total	C	N	O	S	Se	0	0	0
			997	640	158	193	4	2			
1	2	91	Total	C	N	O	S	Se	0	0	0
			716	465	117	128	4	2			
1	E	113	Total	C	N	O	S	Se	0	0	0
			875	565	140	164	4	2			
1	3	104	Total	C	N	O	S	Se	0	0	0
			810	523	132	149	4	2			
1	G	127	Total	C	N	O	S	Se	0	0	0
			995	639	157	193	4	2			
1	o	63	Total	C	N	O	S	Se	0	0	0
			489	319	73	92	3	2			
1	q	47	Total	C	N	O	S	Se	0	0	0
			359	234	57	62	4	2			
1	I	125	Total	C	N	O	S	Se	0	0	0
			979	627	155	191	4	2			
1	4	129	Total	C	N	O	S	Se	0	0	0
			1000	641	158	195	4	2			
1	K	116	Total	C	N	O	S	Se	0	0	0
			905	584	144	171	4	2			
1	5	128	Total	C	N	O	S	Se	0	0	0
			1000	642	158	194	4	2			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	M	124	Total	C	N	O	S	Se	0	0	0
			970	623	154	187	4	2			
1	O	102	Total	C	N	O	S	Se	0	0	0
			812	528	127	151	4	2			
1	a	99	Total	C	N	O	S	Se	0	0	0
			777	507	124	140	4	2			
1	s	102	Total	C	N	O	S	Se	0	0	0
			813	529	130	148	4	2			
1	u	106	Total	C	N	O	S	Se	0	0	0
			831	536	135	154	4	2			
1	c	120	Total	C	N	O	S	Se	0	0	0
			934	603	149	176	4	2			
1	e	126	Total	C	N	O	S	Se	0	0	0
			987	633	156	192	4	2			
1	g	127	Total	C	N	O	S	Se	0	0	0
			994	636	157	195	4	2			
1	i	101	Total	C	N	O	S	Se	0	0	0
			779	506	126	141	4	2			
1	Q	122	Total	C	N	O	S	Se	0	0	0
			945	606	150	183	4	2			
1	S	126	Total	C	N	O	S	Se	0	0	0
			987	633	156	192	4	2			
1	U	101	Total	C	N	O	S	Se	0	0	0
			811	528	129	148	4	2			
1	W	128	Total	C	N	O	S	Se	0	0	0
			1005	647	159	193	4	2			
1	w	49	Total	C	N	O	S	Se	0	0	0
			378	248	59	66	3	2			
1	Y	129	Total	C	N	O	S	Se	0	0	0
			1013	651	161	195	4	2			
1	y	93	Total	C	N	O	S	Se	0	0	0
			738	488	111	133	4	2			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	GLY	-	expression tag	UNP O14713
A	45	PRO	-	expression tag	UNP O14713
A	46	LEU	-	expression tag	UNP O14713
A	47	GLY	-	expression tag	UNP O14713
A	48	SER	-	expression tag	UNP O14713
0	44	GLY	-	expression tag	UNP O14713
0	45	PRO	-	expression tag	UNP O14713

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Chain	Residue	Modelled	Actual	Comment	Reference
0	46	LEU	-	expression tag	UNP O14713
0	47	GLY	-	expression tag	UNP O14713
0	48	SER	-	expression tag	UNP O14713
k	44	GLY	-	expression tag	UNP O14713
k	45	PRO	-	expression tag	UNP O14713
k	46	LEU	-	expression tag	UNP O14713
k	47	GLY	-	expression tag	UNP O14713
k	48	SER	-	expression tag	UNP O14713
m	44	GLY	-	expression tag	UNP O14713
m	45	PRO	-	expression tag	UNP O14713
m	46	LEU	-	expression tag	UNP O14713
m	47	GLY	-	expression tag	UNP O14713
m	48	SER	-	expression tag	UNP O14713
1	44	GLY	-	expression tag	UNP O14713
1	45	PRO	-	expression tag	UNP O14713
1	46	LEU	-	expression tag	UNP O14713
1	47	GLY	-	expression tag	UNP O14713
1	48	SER	-	expression tag	UNP O14713
C	44	GLY	-	expression tag	UNP O14713
C	45	PRO	-	expression tag	UNP O14713
C	46	LEU	-	expression tag	UNP O14713
C	47	GLY	-	expression tag	UNP O14713
C	48	SER	-	expression tag	UNP O14713
2	44	GLY	-	expression tag	UNP O14713
2	45	PRO	-	expression tag	UNP O14713
2	46	LEU	-	expression tag	UNP O14713
2	47	GLY	-	expression tag	UNP O14713
2	48	SER	-	expression tag	UNP O14713
E	44	GLY	-	expression tag	UNP O14713
E	45	PRO	-	expression tag	UNP O14713
E	46	LEU	-	expression tag	UNP O14713
E	47	GLY	-	expression tag	UNP O14713
E	48	SER	-	expression tag	UNP O14713
3	44	GLY	-	expression tag	UNP O14713
3	45	PRO	-	expression tag	UNP O14713
3	46	LEU	-	expression tag	UNP O14713
3	47	GLY	-	expression tag	UNP O14713
3	48	SER	-	expression tag	UNP O14713
G	44	GLY	-	expression tag	UNP O14713
G	45	PRO	-	expression tag	UNP O14713
G	46	LEU	-	expression tag	UNP O14713
G	47	GLY	-	expression tag	UNP O14713

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Chain	Residue	Modelled	Actual	Comment	Reference
G	48	SER	-	expression tag	UNP O14713
o	44	GLY	-	expression tag	UNP O14713
o	45	PRO	-	expression tag	UNP O14713
o	46	LEU	-	expression tag	UNP O14713
o	47	GLY	-	expression tag	UNP O14713
o	48	SER	-	expression tag	UNP O14713
q	44	GLY	-	expression tag	UNP O14713
q	45	PRO	-	expression tag	UNP O14713
q	46	LEU	-	expression tag	UNP O14713
q	47	GLY	-	expression tag	UNP O14713
q	48	SER	-	expression tag	UNP O14713
I	44	GLY	-	expression tag	UNP O14713
I	45	PRO	-	expression tag	UNP O14713
I	46	LEU	-	expression tag	UNP O14713
I	47	GLY	-	expression tag	UNP O14713
I	48	SER	-	expression tag	UNP O14713
4	44	GLY	-	expression tag	UNP O14713
4	45	PRO	-	expression tag	UNP O14713
4	46	LEU	-	expression tag	UNP O14713
4	47	GLY	-	expression tag	UNP O14713
4	48	SER	-	expression tag	UNP O14713
K	44	GLY	-	expression tag	UNP O14713
K	45	PRO	-	expression tag	UNP O14713
K	46	LEU	-	expression tag	UNP O14713
K	47	GLY	-	expression tag	UNP O14713
K	48	SER	-	expression tag	UNP O14713
5	44	GLY	-	expression tag	UNP O14713
5	45	PRO	-	expression tag	UNP O14713
5	46	LEU	-	expression tag	UNP O14713
5	47	GLY	-	expression tag	UNP O14713
5	48	SER	-	expression tag	UNP O14713
M	44	GLY	-	expression tag	UNP O14713
M	45	PRO	-	expression tag	UNP O14713
M	46	LEU	-	expression tag	UNP O14713
M	47	GLY	-	expression tag	UNP O14713
M	48	SER	-	expression tag	UNP O14713
O	44	GLY	-	expression tag	UNP O14713
O	45	PRO	-	expression tag	UNP O14713
O	46	LEU	-	expression tag	UNP O14713
O	47	GLY	-	expression tag	UNP O14713
O	48	SER	-	expression tag	UNP O14713
a	44	GLY	-	expression tag	UNP O14713

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Chain	Residue	Modelled	Actual	Comment	Reference
a	45	PRO	-	expression tag	UNP O14713
a	46	LEU	-	expression tag	UNP O14713
a	47	GLY	-	expression tag	UNP O14713
a	48	SER	-	expression tag	UNP O14713
s	44	GLY	-	expression tag	UNP O14713
s	45	PRO	-	expression tag	UNP O14713
s	46	LEU	-	expression tag	UNP O14713
s	47	GLY	-	expression tag	UNP O14713
s	48	SER	-	expression tag	UNP O14713
u	44	GLY	-	expression tag	UNP O14713
u	45	PRO	-	expression tag	UNP O14713
u	46	LEU	-	expression tag	UNP O14713
u	47	GLY	-	expression tag	UNP O14713
u	48	SER	-	expression tag	UNP O14713
c	44	GLY	-	expression tag	UNP O14713
c	45	PRO	-	expression tag	UNP O14713
c	46	LEU	-	expression tag	UNP O14713
c	47	GLY	-	expression tag	UNP O14713
c	48	SER	-	expression tag	UNP O14713
e	44	GLY	-	expression tag	UNP O14713
e	45	PRO	-	expression tag	UNP O14713
e	46	LEU	-	expression tag	UNP O14713
e	47	GLY	-	expression tag	UNP O14713
e	48	SER	-	expression tag	UNP O14713
g	44	GLY	-	expression tag	UNP O14713
g	45	PRO	-	expression tag	UNP O14713
g	46	LEU	-	expression tag	UNP O14713
g	47	GLY	-	expression tag	UNP O14713
g	48	SER	-	expression tag	UNP O14713
i	44	GLY	-	expression tag	UNP O14713
i	45	PRO	-	expression tag	UNP O14713
i	46	LEU	-	expression tag	UNP O14713
i	47	GLY	-	expression tag	UNP O14713
i	48	SER	-	expression tag	UNP O14713
Q	44	GLY	-	expression tag	UNP O14713
Q	45	PRO	-	expression tag	UNP O14713
Q	46	LEU	-	expression tag	UNP O14713
Q	47	GLY	-	expression tag	UNP O14713
Q	48	SER	-	expression tag	UNP O14713
S	44	GLY	-	expression tag	UNP O14713
S	45	PRO	-	expression tag	UNP O14713
S	46	LEU	-	expression tag	UNP O14713

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Chain	Residue	Modelled	Actual	Comment	Reference
S	47	GLY	-	expression tag	UNP O14713
S	48	SER	-	expression tag	UNP O14713
U	44	GLY	-	expression tag	UNP O14713
U	45	PRO	-	expression tag	UNP O14713
U	46	LEU	-	expression tag	UNP O14713
U	47	GLY	-	expression tag	UNP O14713
U	48	SER	-	expression tag	UNP O14713
W	44	GLY	-	expression tag	UNP O14713
W	45	PRO	-	expression tag	UNP O14713
W	46	LEU	-	expression tag	UNP O14713
W	47	GLY	-	expression tag	UNP O14713
W	48	SER	-	expression tag	UNP O14713
w	44	GLY	-	expression tag	UNP O14713
w	45	PRO	-	expression tag	UNP O14713
w	46	LEU	-	expression tag	UNP O14713
w	47	GLY	-	expression tag	UNP O14713
w	48	SER	-	expression tag	UNP O14713
Y	44	GLY	-	expression tag	UNP O14713
Y	45	PRO	-	expression tag	UNP O14713
Y	46	LEU	-	expression tag	UNP O14713
Y	47	GLY	-	expression tag	UNP O14713
Y	48	SER	-	expression tag	UNP O14713
y	44	GLY	-	expression tag	UNP O14713
y	45	PRO	-	expression tag	UNP O14713
y	46	LEU	-	expression tag	UNP O14713
y	47	GLY	-	expression tag	UNP O14713
y	48	SER	-	expression tag	UNP O14713

- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	l	7	Total	C	N	O	0	0	0
			49	31	9	9			
2	n	11	Total	C	N	O	0	0	0
			79	50	14	15			
2	x	4	Total	C	N	O	0	0	0
			25	15	4	6			
2	D	11	Total	C	N	O	0	0	0
			79	50	14	15			
2	8	8	Total	C	N	O	0	0	0
			55	35	9	11			
2	H	11	Total	C	N	O	0	0	0
			79	50	14	15			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	p	5	Total	C	N	O	0	0	0
			38	25	7	6			
2	B	10	Total	C	N	O	0	0	0
			70	44	12	14			
2	9	8	Total	C	N	O	0	0	0
			54	33	9	12			
2	F	11	Total	C	N	O	0	0	0
			79	50	14	15			
2	r	2	Total	C	N	O	0	0	0
			15	9	3	3			
2	J	11	Total	C	N	O	0	0	0
			79	50	14	15			
2	7	11	Total	C	N	O	0	0	0
			79	50	14	15			
2	L	11	Total	C	N	O	0	0	0
			79	50	14	15			
2	6	11	Total	C	N	O	0	0	0
			79	50	14	15			
2	N	11	Total	C	N	O	0	0	0
			79	50	14	15			
2	P	11	Total	C	N	O	0	0	0
			79	50	14	15			
2	t	8	Total	C	N	O	0	0	0
			58	37	11	10			
2	v	8	Total	C	N	O	0	0	0
			55	35	9	11			
2	b	10	Total	C	N	O	0	0	0
			70	44	12	14			
2	d	11	Total	C	N	O	0	0	0
			79	50	14	15			
2	f	11	Total	C	N	O	0	0	0
			79	50	14	15			
2	h	10	Total	C	N	O	0	0	0
			70	44	12	14			
2	j	4	Total	C	N	O	0	0	0
			27	17	5	5			
2	R	11	Total	C	N	O	0	0	0
			79	50	14	15			
2	T	11	Total	C	N	O	0	0	0
			79	50	14	15			
2	V	10	Total	C	N	O	0	0	0
			70	44	12	14			

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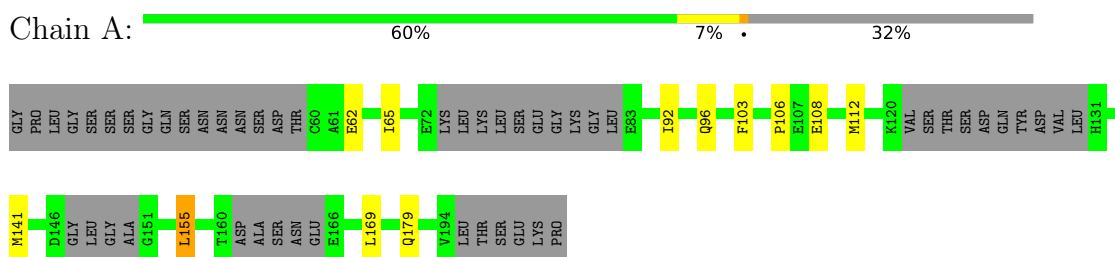
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	X	12	Total	C	N	O	0	0	0
			91	59	15	17			
2	Z	11	Total	C	N	O	0	0	0
			79	50	14	15			
2	z	5	Total	C	N	O	0	0	0
			36	23	6	7			

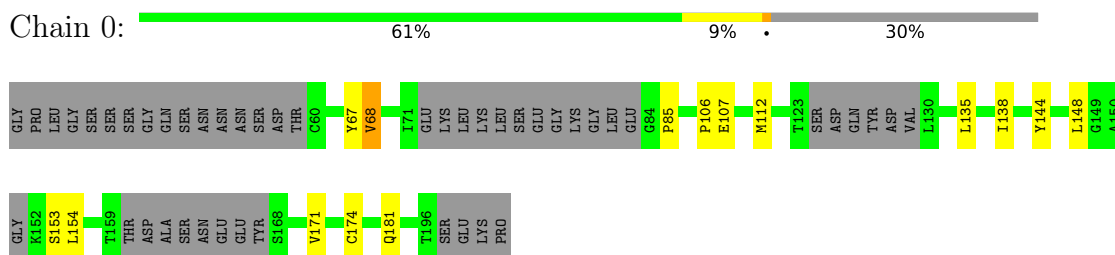
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

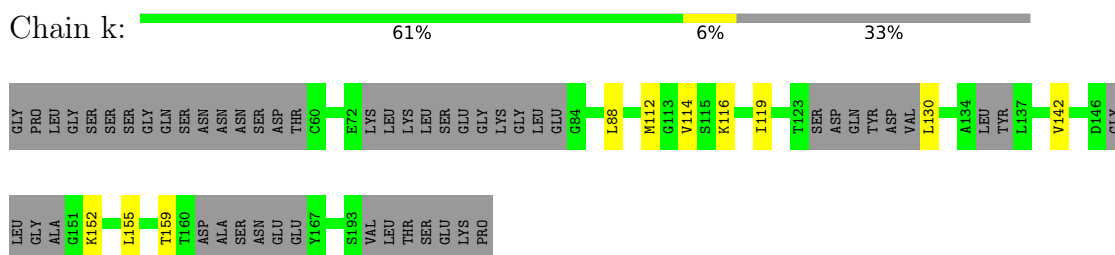
- Molecule 1: Integrin beta-1-binding protein 1



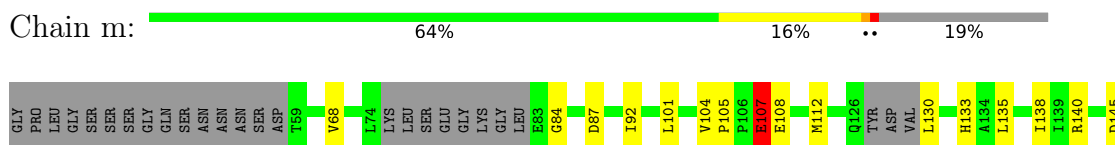
- Molecule 1: Integrin beta-1-binding protein 1



- Molecule 1: Integrin beta-1-binding protein 1



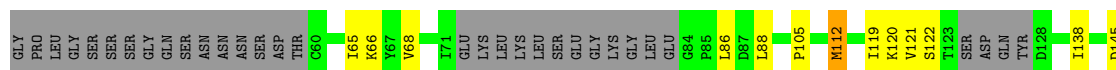
- Molecule 1: Integrin beta-1-binding protein 1





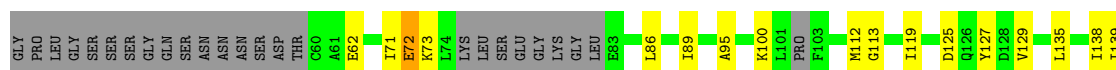
- Molecule 1: Integrin beta-1-binding protein 1

Chain 1: 61% 14% 25%



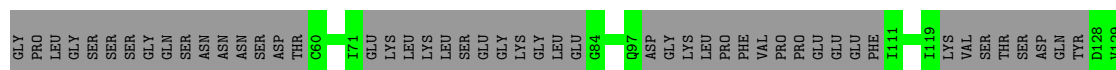
- Molecule 1: Integrin beta-1-binding protein 1

Chain C: 62% 18% 19%



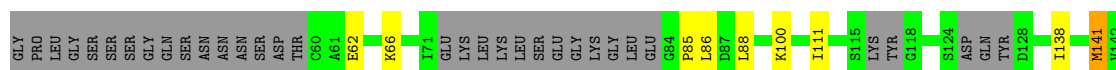
- Molecule 1: Integrin beta-1-binding protein 1

Chain 2: 55% 42%



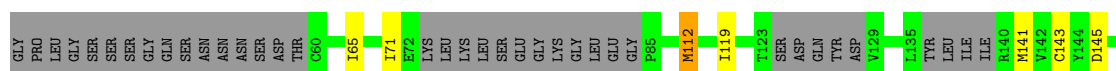
- Molecule 1: Integrin beta-1-binding protein 1

Chain E: 62% 9% 28%



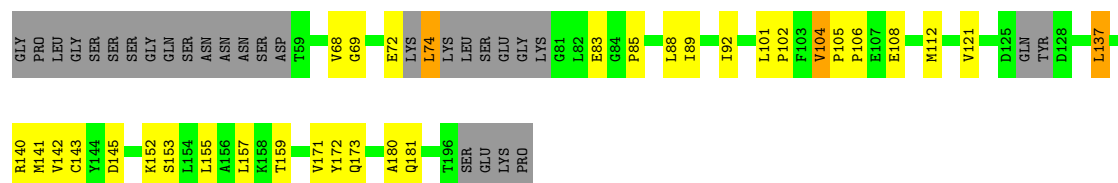
- Molecule 1: Integrin beta-1-binding protein 1

Chain 3: 57% 8% 34%



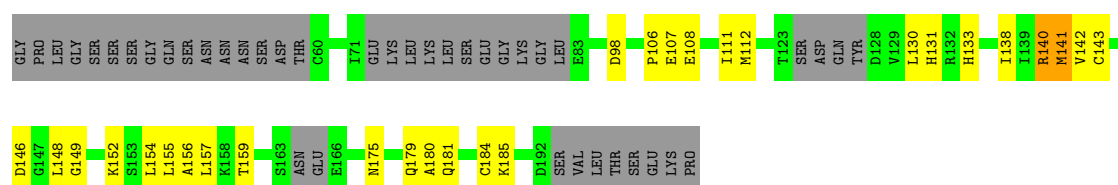
- Molecule 1: Integrin beta-1-binding protein 1

Chain 4: 



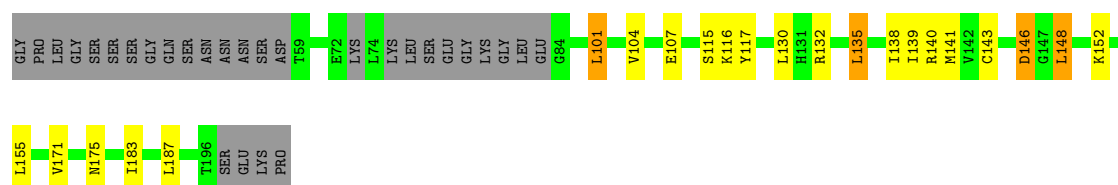
- Molecule 1: Integrin beta-1-binding protein 1

Chain K: 



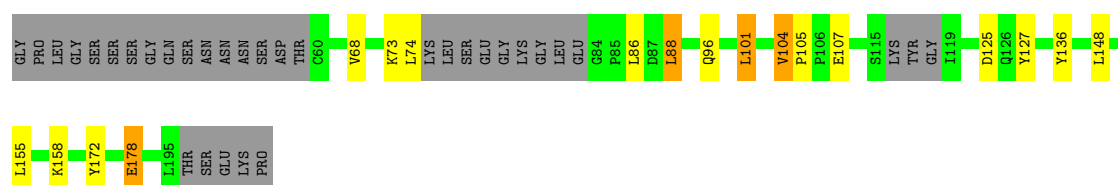
- Molecule 1: Integrin beta-1-binding protein 1

Chain 5: 



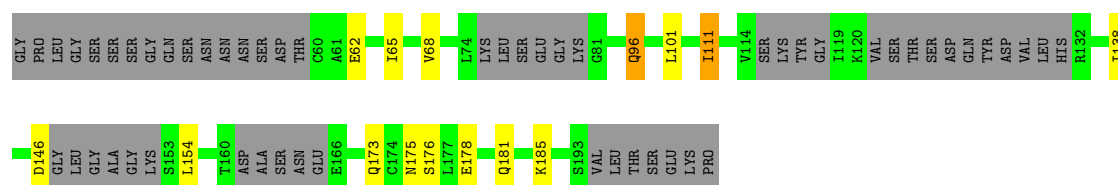
- Molecule 1: Integrin beta-1-binding protein 1

Chain M: 

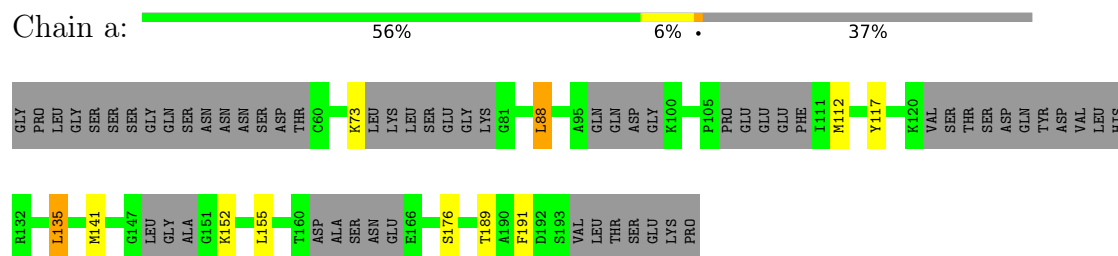


- Molecule 1: Integrin beta-1-binding protein 1

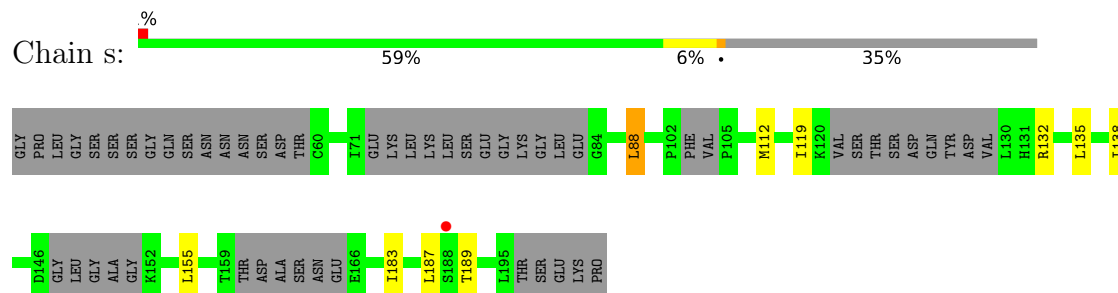
Chain O: 



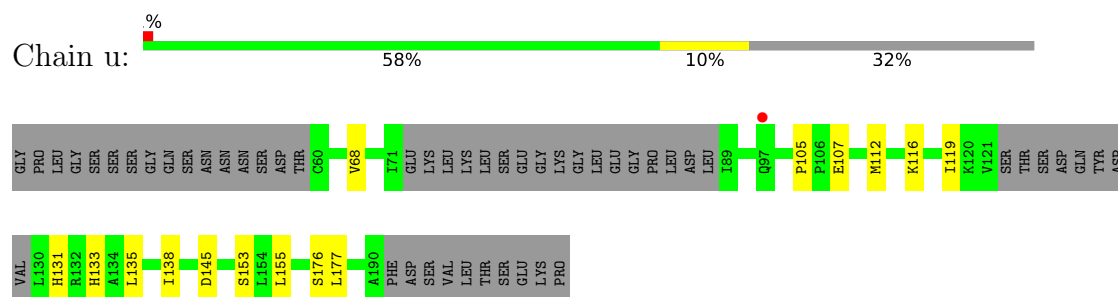
- Molecule 1: Integrin beta-1-binding protein 1



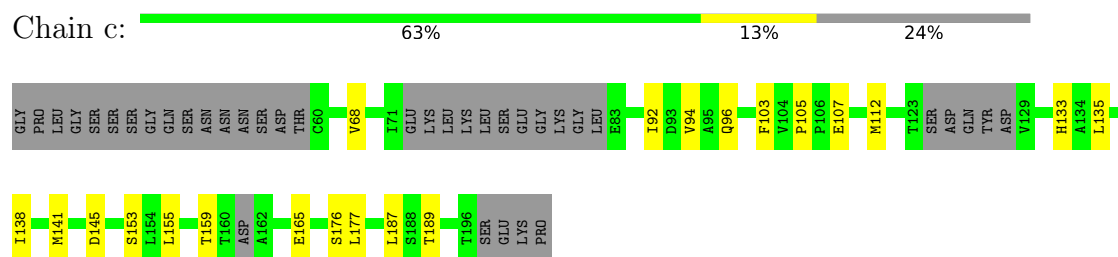
- Molecule 1: Integrin beta-1-binding protein 1



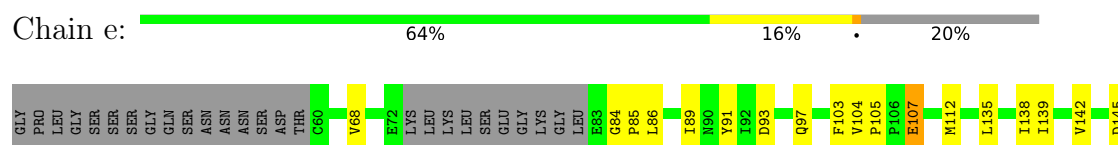
- Molecule 1: Integrin beta-1-binding protein 1



- Molecule 1: Integrin beta-1-binding protein 1



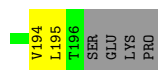
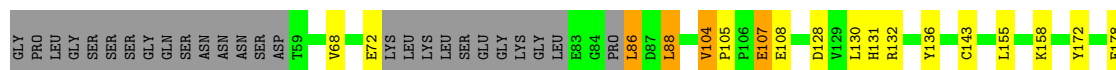
- Molecule 1: Integrin beta-1-binding protein 1





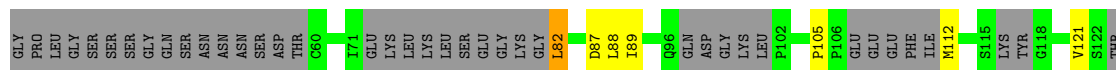
- Molecule 1: Integrin beta-1-binding protein 1

Chain g: 68% 10% 19%



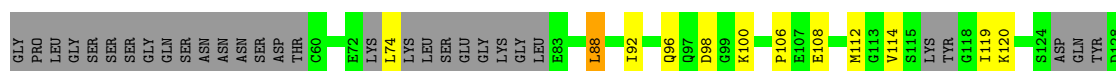
- Molecule 1: Integrin beta-1-binding protein 1

Chain i: 52% 9% 36%



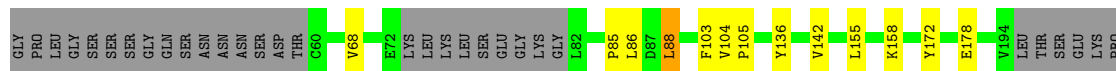
- Molecule 1: Integrin beta-1-binding protein 1

Chain Q: 61% 17% 22%



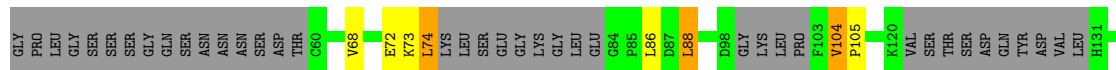
- Molecule 1: Integrin beta-1-binding protein 1

Chain S: 72% 8% 20%



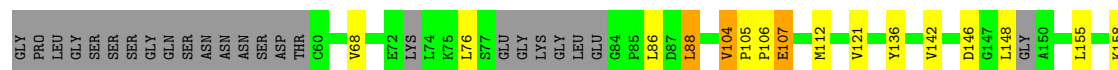
- Molecule 1: Integrin beta-1-binding protein 1

Chain U: 54% 8% 36%

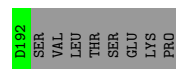
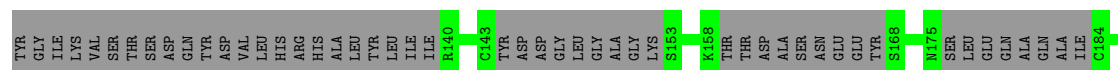
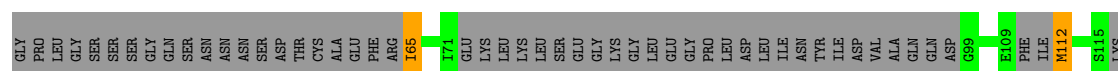




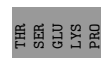
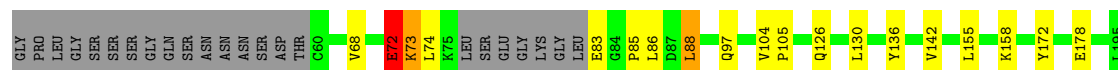
- Molecule 1: Integrin beta-1-binding protein 1



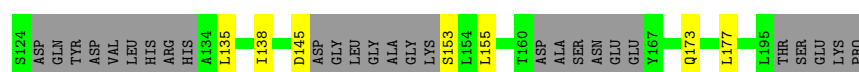
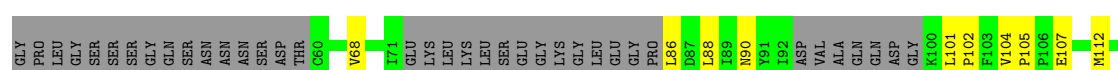
- Molecule 1: Integrin beta-1-binding protein 1



- Molecule 1: Integrin beta-1-binding protein 1



- Molecule 1: Integrin beta-1-binding protein 1

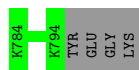


- Molecule 2: Integrin beta-1

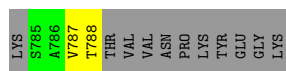




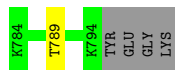
- Molecule 2: Integrin beta-1



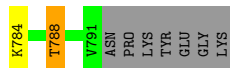
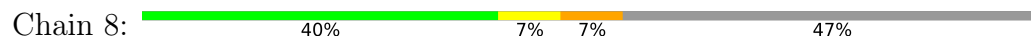
- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1



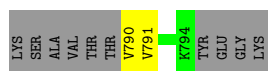
- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1

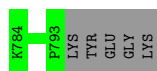


- Molecule 2: Integrin beta-1

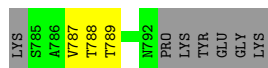
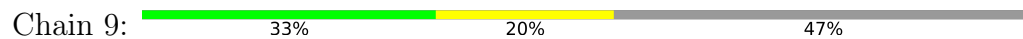


- Molecule 2: Integrin beta-1

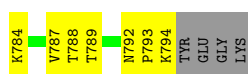




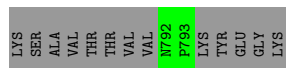
- Molecule 2: Integrin beta-1



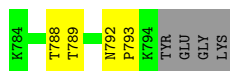
- Molecule 2: Integrin beta-1



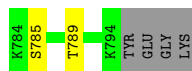
- Molecule 2: Integrin beta-1



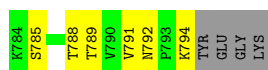
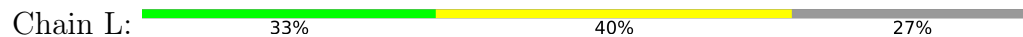
- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1

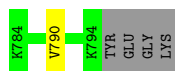


- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1





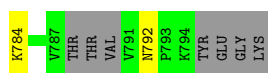
- Molecule 2: Integrin beta-1



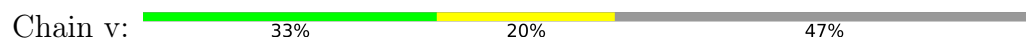
- Molecule 2: Integrin beta-1



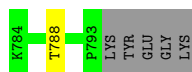
- Molecule 2: Integrin beta-1



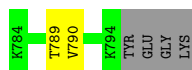
- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1

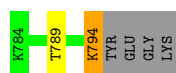


- Molecule 2: Integrin beta-1

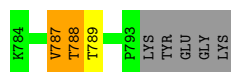


- Molecule 2: Integrin beta-1

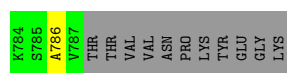




- Molecule 2: Integrin beta-1



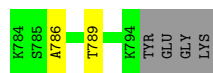
- Molecule 2: Integrin beta-1



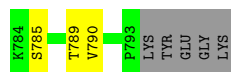
- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1

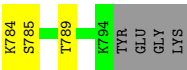


- Molecule 2: Integrin beta-1

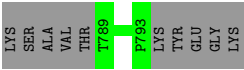


- Molecule 2: Integrin beta-1





● Molecule 2: Integrin beta-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.62Å 122.21Å 135.27Å 89.97° 89.99° 108.11°	Depositor
Resolution (Å)	50.01 – 2.99 50.01 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.01-2.99) 98.4 (50.01-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.251 , 0.312 0.249 , 0.312	Depositor DCC
R_{free} test set	5828 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	67.0	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.458 for h,-h-k,-l 0.458 for -h,-k,l 0.458 for -h,h+k,-l	Xtriage
Reported twinning fraction	0.273 for H, K, L 0.239 for -h,-k,l 0.248 for h,-h-k,-l 0.239 for -H, H+K, -L	Depositor
Outliers	0 of 111606 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	29306	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.51	0/869	0.69	0/1168
1	1	0.53	0/933	0.78	0/1258
1	2	0.53	0/721	0.68	0/966
1	3	0.53	0/820	0.71	0/1100
1	4	0.51	0/1013	0.80	3/1366 (0.2%)
1	5	0.53	0/1015	0.77	0/1371
1	A	0.53	0/856	0.70	0/1149
1	C	0.56	0/1011	0.78	0/1362
1	E	0.52	0/886	0.73	0/1192
1	G	0.50	0/1011	0.74	0/1366
1	I	0.55	0/995	0.80	0/1344
1	K	0.53	0/918	0.75	0/1236
1	M	0.56	0/984	0.78	1/1328 (0.1%)
1	O	0.48	0/821	0.78	0/1101
1	Q	0.51	0/956	0.73	0/1287
1	S	0.50	0/1003	0.72	0/1355
1	U	0.58	1/821 (0.1%)	0.76	1/1100 (0.1%)
1	W	0.50	0/1019	0.71	0/1373
1	Y	0.87	2/1029 (0.2%)	0.82	3/1388 (0.2%)
1	a	0.47	0/784	0.73	0/1046
1	c	0.50	0/947	0.71	0/1276
1	e	0.50	0/1003	0.74	0/1355
1	g	0.49	0/1008	0.73	0/1360
1	i	0.52	0/788	0.71	0/1058
1	k	0.51	0/837	0.70	0/1122
1	m	0.49	0/1005	0.75	1/1355 (0.1%)
1	o	0.42	0/489	0.62	0/651
1	q	0.46	0/359	0.58	0/472
1	s	0.51	0/823	0.69	0/1102
1	u	0.51	0/843	0.71	0/1134
1	w	0.48	0/379	0.69	0/501
1	y	0.60	2/746 (0.3%)	0.70	0/1001
2	6	0.46	0/79	0.81	0/107
2	7	0.50	0/79	0.76	0/107

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	8	0.48	0/54	0.74	0/73
2	9	0.50	0/53	0.65	0/73
2	B	0.53	0/70	0.90	0/96
2	D	0.46	0/79	0.75	0/107
2	F	0.41	0/79	0.76	0/107
2	H	0.44	0/79	0.76	0/107
2	J	0.42	0/79	0.72	0/107
2	L	0.43	0/79	0.89	0/107
2	N	0.48	0/79	0.71	0/107
2	P	0.46	0/79	0.84	0/107
2	R	0.41	0/79	0.70	0/107
2	T	0.49	0/79	0.73	0/107
2	V	0.40	0/70	0.62	0/96
2	X	0.40	0/92	0.73	0/125
2	Z	0.44	0/79	0.71	0/107
2	b	0.47	0/70	0.64	0/96
2	d	0.36	0/79	0.66	0/107
2	f	0.43	0/79	0.67	0/107
2	h	0.50	0/70	0.77	0/96
2	j	0.47	0/26	0.51	0/33
2	l	0.43	0/48	1.00	0/63
2	n	0.39	0/79	0.68	0/107
2	p	0.47	0/38	0.86	0/51
2	r	0.48	0/15	0.25	0/20
2	t	0.43	0/57	0.73	0/74
2	v	0.46	0/55	0.65	0/77
2	x	0.62	0/24	0.47	0/32
2	z	0.53	0/36	0.54	0/50
All	All	0.53	5/29655 (0.0%)	0.74	9/39903 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Y	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	72	GLU	CD-OE2	17.73	1.59	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	72	GLU	C-O	-12.50	1.07	1.24
1	y	173	GLN	CD-NE2	-9.39	1.13	1.33
1	y	173	GLN	CD-OE1	-8.19	1.07	1.23
1	U	72	GLU	CD-OE1	6.33	1.37	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	73	LYS	N-CA-C	9.05	126.14	113.56
1	Y	72	GLU	CA-C-N	-7.78	106.69	121.54
1	Y	72	GLU	C-N-CA	-7.78	106.69	121.54
1	U	73	LYS	N-CA-C	7.43	122.18	111.56
1	Y	72	GLU	O-C-N	-6.45	112.84	122.39
1	4	83	GLU	N-CA-C	6.13	117.76	111.14
1	4	104	VAL	CA-C-N	5.57	126.11	120.38
1	4	104	VAL	C-N-CA	5.57	126.11	120.38
1	m	107	GLU	N-CA-C	5.10	117.57	111.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Y	72	GLU	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	858	0	874	11	0
1	1	919	0	913	14	0
1	2	716	0	736	1	0
1	3	810	0	819	7	0
1	4	1000	0	992	24	0
1	5	1000	0	990	10	1
1	A	844	0	839	6	0
1	C	997	0	988	21	0
1	E	875	0	877	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	995	0	983	17	0
1	I	979	0	961	13	0
1	K	905	0	901	14	0
1	M	970	0	964	26	0
1	O	812	0	814	7	0
1	Q	945	0	937	24	0
1	S	987	0	972	6	0
1	U	811	0	813	10	0
1	W	1005	0	1001	20	0
1	Y	1013	0	1009	8	1
1	a	777	0	794	5	0
1	c	934	0	937	9	0
1	e	987	0	972	22	0
1	g	994	0	978	32	0
1	i	779	0	789	13	0
1	k	827	0	829	2	0
1	m	991	0	987	29	0
1	o	489	0	481	7	0
1	q	359	0	363	0	0
1	s	813	0	821	7	0
1	u	831	0	834	7	0
1	w	378	0	387	2	0
1	y	738	0	759	5	0
2	6	79	0	89	1	0
2	7	79	0	89	3	0
2	8	55	0	63	1	0
2	9	54	0	56	3	0
2	B	70	0	76	0	0
2	D	79	0	89	1	0
2	F	79	0	89	5	0
2	H	79	0	89	8	0
2	J	79	0	89	3	0
2	L	79	0	89	6	0
2	N	79	0	89	1	0
2	P	79	0	89	1	0
2	R	79	0	89	4	0
2	T	79	0	89	3	0
2	V	70	0	76	2	0
2	X	91	0	98	2	0
2	Z	79	0	89	3	0
2	b	70	0	76	1	0
2	d	79	0	89	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	f	79	0	89	2	0
2	h	70	0	76	2	0
2	j	27	0	31	1	0
2	l	49	0	52	0	0
2	n	79	0	89	0	0
2	p	38	0	43	1	0
2	r	15	0	12	0	0
2	t	58	0	65	1	0
2	v	55	0	58	1	0
2	x	25	0	25	1	0
2	z	36	0	37	0	0
All	All	29306	0	29493	329	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (329) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:107:GLU:CG	1:M:105:PRO:O	1.73	1.36
1:m:107:GLU:OE2	1:M:104:VAL:HG12	1.26	1.31
1:e:107:GLU:N	1:g:72:GLU:OE2	1.69	1.23
1:g:107:GLU:CD	1:W:105:PRO:O	1.82	1.20
1:g:107:GLU:OE2	1:W:105:PRO:O	1.65	1.15
1:m:107:GLU:CD	1:M:104:VAL:HG12	1.73	1.13
1:4:105:PRO:HD2	1:4:173:GLN:NE2	1.65	1.11
1:m:107:GLU:CD	1:M:105:PRO:O	1.95	1.09
1:C:127:TYR:HB3	1:Q:100:LYS:NZ	1.74	1.02
1:m:107:GLU:HG2	1:M:105:PRO:O	1.57	1.00
1:e:107:GLU:HB2	1:g:72:GLU:CD	1.87	0.99
1:0:107:GLU:O	1:0:107:GLU:HG3	1.61	0.97
1:e:107:GLU:HB2	1:g:72:GLU:OE2	1.68	0.94
1:4:105:PRO:CD	1:4:173:GLN:NE2	2.31	0.93
1:m:107:GLU:HG3	1:M:105:PRO:O	1.68	0.92
1:i:155:LEU:HB2	1:i:172:TYR:O	1.73	0.88
1:C:127:TYR:HB3	1:Q:100:LYS:HZ3	1.37	0.87
1:m:107:GLU:OE1	1:M:104:VAL:HB	1.73	0.87
1:4:105:PRO:HD2	1:4:173:GLN:HE22	1.39	0.84
1:U:181:GLN:NE2	2:V:785:SER:OG	2.12	0.82
1:e:103:PHE:CG	1:g:132:ARG:HD2	2.14	0.81
2:L:792:ASN:O	2:L:794:LYS:HA	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:104:VAL:CG2	1:W:148:LEU:HB3	2.12	0.79
1:m:107:GLU:OE2	1:M:104:VAL:CG1	2.21	0.79
1:m:107:GLU:CD	1:M:104:VAL:CG1	2.55	0.78
1:s:189:THR:HG21	1:u:176:SER:HB2	1.66	0.78
1:0:107:GLU:HG2	1:u:116:LYS:HD2	1.66	0.77
1:K:181:GLN:HG2	2:L:788:THR:HG21	1.66	0.77
1:Y:72:GLU:O	1:Y:73:LYS:HG3	1.85	0.77
1:g:107:GLU:CD	1:W:105:PRO:C	2.51	0.77
1:g:104:VAL:HG23	1:W:148:LEU:HB3	1.67	0.77
1:Y:72:GLU:O	1:Y:73:LYS:CG	2.32	0.76
1:e:103:PHE:HB2	1:g:132:ARG:HB2	1.68	0.76
1:e:104:VAL:HG21	1:g:131:HIS:HA	1.66	0.76
1:m:107:GLU:OE1	1:M:104:VAL:CB	2.33	0.75
1:Y:72:GLU:O	1:Y:73:LYS:CB	2.29	0.75
1:C:127:TYR:HB3	1:Q:100:LYS:HZ1	1.48	0.74
1:e:107:GLU:CB	1:g:72:GLU:OE2	2.34	0.74
1:G:85:PRO:HB3	2:H:789:THR:HG21	1.68	0.73
1:c:187:LEU:HB3	2:d:790:VAL:HG11	1.70	0.72
1:Q:189:THR:HG23	1:U:178:GLU:HG3	1.70	0.72
1:I:141:MSE:HE2	1:I:187:LEU:HD22	1.72	0.71
1:i:173:GLN:HG3	1:i:174:CYS:N	2.03	0.71
1:5:101:LEU:HD11	1:5:171:VAL:HG21	1.71	0.71
1:e:107:GLU:CA	1:g:72:GLU:OE2	2.38	0.70
1:Q:189:THR:HG21	1:U:176:SER:HB2	1.73	0.70
1:g:86:LEU:HD11	1:i:144:TYR:HB2	1.74	0.70
1:I:141:MSE:HE3	1:I:184:CYS:HA	1.74	0.68
1:g:107:GLU:OE2	1:W:105:PRO:C	2.35	0.68
1:0:107:GLU:CG	1:u:116:LYS:HD2	2.24	0.67
2:H:787:VAL:HB	2:F:787:VAL:HB	1.77	0.66
1:o:120:LYS:HE3	1:s:132:ARG:HH22	1.61	0.66
1:0:153:SER:HB3	1:0:174:CYS:HB2	1.78	0.66
1:m:107:GLU:OE1	1:M:104:VAL:CG1	2.45	0.65
1:4:112:MSE:HG3	1:4:121:VAL:HG22	1.78	0.64
1:m:104:VAL:HG13	1:M:104:VAL:HG22	1.78	0.64
1:4:141:MSE:HE2	1:4:155:LEU:HD21	1.80	0.63
1:W:142:VAL:HG22	2:X:789:THR:HG22	1.78	0.63
1:Q:114:VAL:HG22	1:Q:119:ILE:HG13	1.81	0.63
1:E:66:LYS:HB2	1:E:173:GLN:HB3	1.81	0.62
1:C:141:MSE:HE3	1:C:184:CYS:HA	1.81	0.62
1:C:142:VAL:HG22	2:D:789:THR:HG23	1.81	0.62
1:U:74:LEU:HD12	1:U:167:TYR:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:103:PHE:CG	1:g:132:ARG:CD	2.83	0.61
1:0:107:GLU:O	1:0:107:GLU:CG	2.43	0.61
1:K:148:LEU:HB3	1:Q:149:GLY:HA3	1.83	0.60
1:i:150:ALA:HB1	1:y:104:VAL:HG22	1.82	0.60
1:e:103:PHE:CD2	1:g:132:ARG:HD3	2.36	0.60
1:C:125:ASP:C	1:C:127:TYR:H	2.10	0.60
1:4:89:ILE:HD11	1:4:142:VAL:HG11	1.85	0.59
1:i:152:LYS:HB3	1:i:173:GLN:OE1	2.03	0.59
1:K:140:ARG:HG2	2:L:791:VAL:HG12	1.85	0.59
1:g:107:GLU:CG	1:W:105:PRO:O	2.50	0.59
1:Q:189:THR:HG21	1:U:176:SER:CB	2.33	0.58
1:m:104:VAL:HG21	1:M:148:LEU:HD13	1.86	0.58
1:4:105:PRO:CD	1:4:173:GLN:HE21	2.13	0.58
1:4:137:LEU:HD12	1:4:159:THR:HB	1.86	0.58
1:Q:119:ILE:HD13	1:Q:138:ILE:HD13	1.86	0.58
2:R:788:THR:HA	2:T:786:ALA:H	1.70	0.57
1:G:141:MSE:HE3	1:G:157:LEU:HD13	1.87	0.57
1:K:185:LYS:HB3	1:O:178:GLU:O	2.05	0.57
1:S:85:PRO:HB3	2:T:789:THR:HG21	1.86	0.56
1:3:141:MSE:HG3	1:3:157:LEU:HG	1.88	0.56
1:G:68:VAL:HG22	1:G:105:PRO:HG3	1.88	0.56
1:g:107:GLU:OE2	1:W:104:VAL:HG12	2.06	0.55
1:C:185:LYS:HB3	1:G:178:GLU:HB3	1.87	0.55
1:1:145:ASP:HA	1:1:153:SER:HA	1.88	0.55
1:c:133:HIS:HD2	1:c:159:THR:HG21	1.72	0.55
1:g:107:GLU:OE2	1:W:105:PRO:N	2.39	0.54
1:E:138:ILE:HA	1:E:159:THR:HG22	1.88	0.54
1:A:62:GLU:HB2	1:E:62:GLU:HB2	1.89	0.54
1:4:85:PRO:HB3	2:7:789:THR:HG21	1.90	0.54
1:O:62:GLU:HG2	1:O:111:ILE:HG22	1.89	0.54
1:4:85:PRO:HG3	1:4:140:ARG:CZ	2.37	0.54
1:g:107:GLU:OE1	1:W:106:PRO:O	2.26	0.54
1:m:107:GLU:HG2	1:M:105:PRO:C	2.32	0.53
1:K:141:MSE:HE1	1:K:184:CYS:HA	1.89	0.53
1:s:119:ILE:HD11	1:s:187:LEU:HD21	1.90	0.53
1:Y:142:VAL:HG22	2:Z:789:THR:HG22	1.89	0.53
1:C:73:LYS:HE2	1:I:166:GLU:HG3	1.89	0.53
1:G:142:VAL:HG22	2:H:789:THR:HG22	1.90	0.52
1:I:85:PRO:HB3	2:J:789:THR:HG21	1.91	0.52
1:e:142:VAL:HG22	2:f:789:THR:HG22	1.90	0.52
1:e:152:LYS:HD3	1:e:175:ASN:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:143:CYS:HB3	1:G:155:LEU:HD23	1.89	0.52
1:M:96:GLN:HA	1:M:101:LEU:O	2.09	0.52
2:H:792:ASN:O	2:H:794:LYS:N	2.40	0.52
2:F:792:ASN:O	2:F:794:LYS:N	2.42	0.52
1:E:86:LEU:HD11	1:G:89:ILE:HG21	1.92	0.52
1:a:176:SER:OG	1:c:189:THR:HG23	2.10	0.52
1:m:92:ILE:HG23	1:m:101:LEU:HD13	1.92	0.51
1:o:140:ARG:HG3	2:p:791:VAL:HG12	1.92	0.51
1:w:65:ILE:HG21	1:w:112:MSE:HE2	1.92	0.51
1:g:143:CYS:SG	2:h:788:THR:HG23	2.50	0.51
1:Q:142:VAL:HG22	2:R:789:THR:HG23	1.91	0.51
1:C:62:GLU:HB2	1:G:62:GLU:HB2	1.92	0.51
1:1:65:ILE:HD13	1:1:172:TYR:HD2	1.76	0.51
1:C:113:GLY:O	1:C:119:ILE:HA	2.11	0.51
1:G:109:GLU:CD	1:G:109:GLU:H	2.18	0.51
1:e:86:LEU:HA	1:e:89:ILE:HD12	1.92	0.51
1:Q:135:LEU:HA	1:Q:138:ILE:HD12	1.93	0.50
1:W:112:MSE:HG3	1:W:121:VAL:HG22	1.93	0.50
1:C:71:ILE:HD11	1:C:95:ALA:CB	2.42	0.50
1:4:88:LEU:O	1:4:92:ILE:HD12	2.11	0.50
1:4:143:CYS:SG	1:4:180:ALA:HB3	2.51	0.50
1:W:184:CYS:O	2:X:790:VAL:HG21	2.12	0.50
1:1:66:LYS:HE2	1:1:105:PRO:HG2	1.93	0.50
1:m:104:VAL:CG1	1:M:104:VAL:HG22	2.42	0.50
1:G:138:ILE:HA	1:G:159:THR:HG22	1.93	0.50
1:4:68:VAL:HB	1:4:171:VAL:HG13	1.94	0.50
1:5:132:ARG:HB3	1:S:103:PHE:HB2	1.94	0.50
2:L:792:ASN:O	2:L:794:LYS:CA	2.56	0.49
1:e:103:PHE:CD1	1:g:132:ARG:HD2	2.45	0.49
1:0:85:PRO:HB3	2:9:789:THR:HG21	1.94	0.49
1:M:88:LEU:HD21	1:M:158:LYS:HB2	1.95	0.49
1:Q:106:PRO:HB2	1:Q:108:GLU:HG2	1.95	0.49
1:S:88:LEU:HD21	1:S:158:LYS:HB2	1.95	0.49
1:1:86:LEU:HD22	1:4:89:ILE:HG21	1.94	0.49
1:4:72:GLU:C	1:4:74:LEU:HD23	2.38	0.49
1:e:103:PHE:CD2	1:g:132:ARG:CD	2.96	0.48
1:Q:181:GLN:HG2	2:R:788:THR:HG21	1.93	0.48
1:0:67:TYR:O	1:0:106:PRO:HD2	2.13	0.48
1:k:114:VAL:HG22	1:k:119:ILE:HG12	1.96	0.48
1:C:86:LEU:HA	1:C:89:ILE:HD12	1.94	0.48
1:W:88:LEU:HD21	1:W:158:LYS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:105:PRO:HG3	1:i:173:GLN:HE21	1.79	0.48
1:A:92:ILE:O	1:A:96:GLN:HB2	2.13	0.48
2:h:787:VAL:HG23	2:j:786:ALA:HB3	1.96	0.48
1:C:155:LEU:HB3	1:C:172:TYR:HB2	1.94	0.48
1:Y:88:LEU:HD21	1:Y:158:LYS:HB2	1.95	0.48
1:C:152:LYS:HD2	1:C:175:ASN:HA	1.96	0.48
1:Q:187:LEU:O	1:Q:191:PHE:HB2	2.14	0.48
1:S:142:VAL:HG22	2:T:789:THR:HG22	1.96	0.48
1:A:106:PRO:HB2	1:A:108:GLU:HG2	1.95	0.48
1:1:88:LEU:HD13	1:1:158:LYS:HE3	1.96	0.48
2:J:788:THR:HG22	2:L:785:SER:HA	1.95	0.48
1:g:107:GLU:OE1	1:W:106:PRO:C	2.57	0.48
1:K:138:ILE:HA	1:K:159:THR:HG22	1.94	0.47
1:A:112:MSE:HE1	1:A:155:LEU:HD22	1.95	0.47
1:m:152:LYS:HG3	1:m:175:ASN:HA	1.95	0.47
1:m:153:SER:OG	1:m:177:LEU:HA	2.15	0.47
1:4:105:PRO:HD2	1:4:173:GLN:HE21	1.66	0.47
1:g:88:LEU:HD21	1:g:158:LYS:HB2	1.95	0.47
1:K:106:PRO:C	1:K:108:GLU:H	2.23	0.47
1:4:142:VAL:HG22	2:7:789:THR:HG22	1.97	0.47
1:s:135:LEU:HA	1:s:138:ILE:HD12	1.97	0.47
1:m:108:GLU:HB3	1:M:107:GLU:OE1	2.14	0.47
1:g:194:VAL:HG23	1:g:195:LEU:HD12	1.97	0.47
1:i:170:TRP:HB2	1:i:172:TYR:HE1	1.79	0.47
1:U:88:LEU:HD21	1:U:158:LYS:HB2	1.95	0.47
1:y:153:SER:OG	1:y:177:LEU:HA	2.15	0.47
1:e:194:VAL:HG23	1:e:195:LEU:HD12	1.96	0.47
1:U:184:CYS:O	2:V:790:VAL:HG21	2.14	0.47
1:1:68:VAL:HA	1:1:105:PRO:HB3	1.97	0.46
1:c:153:SER:OG	1:c:177:LEU:HA	2.14	0.46
1:O:96:GLN:HG2	1:O:101:LEU:HD12	1.97	0.46
1:m:187:LEU:HD23	1:m:191:PHE:HE2	1.79	0.46
1:4:69:GLY:HA3	1:4:101:LEU:HD22	1.96	0.46
1:e:148:LEU:O	1:g:128:ASP:HA	2.15	0.46
1:e:153:SER:OG	1:e:177:LEU:HA	2.14	0.46
1:Q:120:LYS:HE2	1:Q:129:VAL:HG13	1.98	0.46
1:m:84:GLY:HA3	1:m:87:ASP:HB2	1.97	0.46
1:4:145:ASP:HA	1:4:153:SER:HA	1.96	0.46
1:I:146:ASP:OD1	1:I:146:ASP:N	2.41	0.46
1:1:119:ILE:HD11	1:1:187:LEU:HD13	1.98	0.46
1:3:65:ILE:HG12	1:3:112:MSE:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:PRO:HG2	1:G:86:LEU:HD12	1.97	0.46
1:m:108:GLU:HB3	1:M:107:GLU:OE2	2.15	0.46
1:I:185:LYS:HG3	1:M:178:GLU:HB3	1.97	0.46
1:W:146:ASP:HB2	1:W:148:LEU:HD12	1.98	0.46
2:H:789:THR:O	2:F:784:LYS:HB3	2.16	0.46
1:u:153:SER:OG	1:u:177:LEU:HA	2.15	0.46
1:i:172:TYR:CD1	1:i:172:TYR:N	2.83	0.46
1:K:142:VAL:HB	1:K:156:ALA:HB3	1.97	0.46
1:I:139:ILE:HD12	1:I:158:LYS:HG2	1.97	0.46
1:U:155:LEU:HB3	1:U:172:TYR:HB2	1.98	0.46
1:Y:155:LEU:HB3	1:Y:172:TYR:HB2	1.98	0.45
1:K:149:GLY:HA3	1:Q:148:LEU:HB3	1.98	0.45
1:A:141:MSE:HE3	1:A:155:LEU:HD11	1.98	0.45
1:1:138:ILE:HG12	1:1:157:LEU:HD21	1.98	0.45
1:M:155:LEU:HB3	1:M:172:TYR:HB2	1.97	0.45
1:O:175:ASN:O	1:O:176:SER:HB3	2.16	0.45
1:O:135:LEU:HA	1:O:138:ILE:HD12	1.98	0.45
1:k:142:VAL:O	1:k:155:LEU:HA	2.16	0.45
1:K:146:ASP:HB3	1:K:154:LEU:HG	1.99	0.45
1:O:181:GLN:O	1:O:185:LYS:HG2	2.17	0.45
1:S:155:LEU:HB3	1:S:172:TYR:HB2	1.98	0.45
1:Y:85:PRO:HB3	2:Z:789:THR:HG21	1.99	0.45
1:5:187:LEU:HD23	2:6:790:VAL:HG11	1.99	0.45
1:5:139:ILE:HG22	1:5:140:ARG:HG3	1.98	0.45
1:a:189:THR:HG21	1:c:176:SER:HB2	1.99	0.45
1:g:155:LEU:HB3	1:g:172:TYR:HB2	1.98	0.45
1:E:153:SER:HB3	1:E:174:CYS:HB2	1.99	0.44
1:o:194:VAL:HG23	1:o:195:LEU:HD12	1.99	0.44
1:e:85:PRO:HG2	1:e:86:LEU:HD12	1.98	0.44
1:I:119:ILE:HD12	1:I:157:LEU:HD21	1.99	0.44
1:3:181:GLN:HG2	2:8:788:THR:HG21	2.00	0.44
1:5:146:ASP:OD1	1:5:146:ASP:N	2.50	0.44
1:W:155:LEU:HB3	1:W:172:TYR:HB2	1.99	0.44
1:G:143:CYS:HA	1:G:154:LEU:O	2.17	0.44
1:i:176:SER:OG	1:i:179:GLN:HB2	2.18	0.44
1:m:108:GLU:HB3	1:M:107:GLU:CD	2.43	0.44
1:a:141:MSE:HE2	1:a:155:LEU:HD23	2.00	0.44
1:4:85:PRO:O	1:4:89:ILE:HD12	2.16	0.44
1:e:139:ILE:HG23	2:f:794:LYS:HD2	1.98	0.44
1:Y:68:VAL:HA	1:Y:105:PRO:HB3	1.99	0.44
1:O:181:GLN:HG2	2:9:788:THR:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:142:VAL:HG22	2:L:789:THR:HG22	2.00	0.44
1:g:68:VAL:HA	1:g:105:PRO:HB3	2.00	0.44
1:m:84:GLY:H	1:m:140:ARG:NH1	2.16	0.44
1:a:135:LEU:HD21	1:a:191:PHE:HA	1.99	0.44
1:e:68:VAL:HG22	1:e:105:PRO:HB3	2.00	0.44
1:g:104:VAL:HG21	1:W:148:LEU:HB3	1.97	0.44
1:2:179:GLN:HG2	1:3:186:VAL:HG22	1.98	0.43
1:o:157:LEU:HB2	1:o:170:TRP:HB2	2.00	0.43
1:Q:150:ALA:O	1:Q:152:LYS:N	2.50	0.43
1:I:68:VAL:HA	1:I:105:PRO:HB3	1.98	0.43
1:0:68:VAL:HB	1:0:171:VAL:HB	2.00	0.43
1:c:135:LEU:HA	1:c:138:ILE:HD12	2.01	0.43
1:Q:181:GLN:HG2	2:R:788:THR:CG2	2.47	0.43
1:0:144:TYR:HB3	2:9:787:VAL:HG13	1.99	0.43
1:U:68:VAL:HA	1:U:105:PRO:HB3	2.00	0.43
1:m:84:GLY:H	1:m:140:ARG:HH12	1.67	0.43
1:4:106:PRO:C	1:4:108:GLU:H	2.26	0.43
2:N:785:SER:HA	2:P:788:THR:HA	1.99	0.43
1:3:155:LEU:HB2	1:3:172:TYR:HB2	1.99	0.43
1:u:119:ILE:HB	1:u:133:HIS:CD2	2.54	0.43
1:1:153:SER:HB3	1:1:174:CYS:HB2	2.00	0.43
2:H:785:SER:HA	2:F:788:THR:HG22	2.00	0.43
1:u:135:LEU:HA	1:u:138:ILE:HD12	2.01	0.43
1:c:68:VAL:HG22	1:c:105:PRO:HB3	2.00	0.43
1:1:120:LYS:HE3	1:1:122:SER:HB3	2.01	0.42
1:o:86:LEU:HA	1:o:89:ILE:HD12	2.01	0.42
2:J:792:ASN:HA	2:J:793:PRO:HD3	1.85	0.42
1:O:146:ASP:H	1:O:154:LEU:HD23	1.83	0.42
1:m:194:VAL:C	1:m:196:THR:H	2.27	0.42
2:x:788:THR:HB	2:7:785:SER:HA	2.00	0.42
1:s:138:ILE:O	2:t:792:ASN:HB3	2.19	0.42
1:S:68:VAL:HA	1:S:105:PRO:HB3	2.00	0.42
1:G:139:ILE:HD12	1:G:158:LYS:HG2	2.02	0.42
1:Q:191:PHE:O	1:Q:194:VAL:HG22	2.19	0.42
1:C:71:ILE:HD11	1:C:95:ALA:HB1	2.00	0.42
1:Q:119:ILE:N	1:Q:119:ILE:HD12	2.34	0.42
1:1:112:MSE:HG3	1:1:121:VAL:HG22	2.02	0.42
1:C:86:LEU:HD23	1:C:89:ILE:HD12	2.01	0.42
1:G:142:VAL:HB	1:G:156:ALA:HB3	2.02	0.42
1:I:135:LEU:HA	1:I:138:ILE:HD12	2.01	0.42
1:W:68:VAL:HA	1:W:105:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:68:VAL:HG22	1:y:105:PRO:HB3	2.01	0.42
1:G:125:ASP:C	1:G:127:TYR:H	2.28	0.42
1:M:68:VAL:HA	1:M:105:PRO:HB3	2.01	0.42
1:s:155:LEU:HD11	1:s:183:ILE:HD12	2.01	0.42
1:i:82:LEU:N	1:i:87:ASP:HB3	2.35	0.42
1:A:65:ILE:HG12	1:A:112:MSE:HB2	2.00	0.42
1:3:143:CYS:HB3	1:3:155:LEU:HD23	2.02	0.42
1:e:135:LEU:HA	1:e:138:ILE:HD12	2.01	0.42
1:C:135:LEU:HA	1:C:138:ILE:HD12	2.01	0.42
1:4:143:CYS:SG	1:4:181:GLN:HG3	2.60	0.42
1:M:125:ASP:HB2	1:M:127:TYR:HB2	2.02	0.42
1:u:68:VAL:HG22	1:u:105:PRO:HB3	2.01	0.42
1:w:65:ILE:HG12	1:w:112:MSE:HG2	2.01	0.42
1:y:101:LEU:HA	1:y:102:PRO:HD3	1.95	0.42
1:y:135:LEU:HA	1:y:138:ILE:HD12	2.01	0.42
1:m:135:LEU:HA	1:m:138:ILE:HD12	2.01	0.41
1:m:105:PRO:O	1:M:104:VAL:HG11	2.19	0.41
1:1:153:SER:O	1:1:173:GLN:HG3	2.19	0.41
1:G:85:PRO:CB	2:H:789:THR:HG21	2.45	0.41
1:5:115:SER:C	1:5:117:TYR:H	2.28	0.41
1:Q:135:LEU:HD11	1:Q:191:PHE:HA	2.01	0.41
2:H:786:ALA:HB2	2:F:789:THR:HG22	2.02	0.41
1:s:88:LEU:HD12	1:s:88:LEU:HA	1.94	0.41
1:m:68:VAL:HG22	1:m:105:PRO:HB3	2.01	0.41
1:C:125:ASP:C	1:C:127:TYR:N	2.77	0.41
1:I:129:VAL:HB	1:I:132:ARG:NH1	2.36	0.41
1:5:135:LEU:HA	1:5:138:ILE:HD12	2.02	0.41
1:O:68:VAL:HG22	1:O:173:GLN:HB2	2.02	0.41
2:b:788:THR:HG22	2:Z:785:SER:HA	2.02	0.41
1:c:96:GLN:HB3	1:c:103:PHE:CZ	2.55	0.41
1:K:130:LEU:HB3	1:K:131:HIS:H	1.55	0.41
1:K:143:CYS:SG	1:K:180:ALA:CB	3.09	0.41
1:c:141:MSE:O	2:d:789:THR:HA	2.20	0.41
1:C:178:GLU:O	1:G:185:LYS:HB3	2.21	0.41
1:E:141:MSE:SE	1:E:184:CYS:SG	3.29	0.41
1:Q:92:ILE:O	1:Q:96:GLN:HB2	2.21	0.41
1:5:143:CYS:HB3	1:5:155:LEU:HD12	2.03	0.41
1:4:157:LEU:HD12	1:4:172:TYR:HE1	1.86	0.41
1:Q:88:LEU:HD12	1:Q:88:LEU:HA	1.98	0.41
1:C:159:THR:OG1	1:C:170:TRP:NE1	2.54	0.41
1:I:141:MSE:SE	1:I:155:LEU:HD21	2.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:101:LEU:HA	1:4:102:PRO:HD3	1.92	0.41
1:a:88:LEU:HD12	1:a:88:LEU:HA	1.97	0.41
1:g:108:GLU:HG2	1:W:107:GLU:OE2	2.21	0.41
1:i:121:VAL:HB	1:i:131:HIS:HB2	2.03	0.41
1:C:72:GLU:H	1:C:72:GLU:HG2	1.72	0.40
1:3:145:ASP:HB2	1:3:177:LEU:HD22	2.03	0.40
1:5:148:LEU:HD13	1:5:148:LEU:HA	1.91	0.40
1:5:152:LYS:HD3	1:5:175:ASN:O	2.21	0.40
1:M:104:VAL:HA	1:M:105:PRO:HD2	1.89	0.40
2:v:792:ASN:HA	2:v:793:PRO:HD3	1.93	0.40
1:E:85:PRO:HA	1:E:88:LEU:HD13	2.02	0.40
1:K:152:LYS:HE2	1:K:175:ASN:HA	2.04	0.40
1:i:157:LEU:HB3	1:i:170:TRP:HD1	1.86	0.40
1:U:104:VAL:HA	1:U:105:PRO:HD2	1.89	0.40
1:1:65:ILE:HD13	1:1:172:TYR:CD2	2.56	0.40
1:o:145:ASP:HB2	1:o:177:LEU:HD22	2.03	0.40
1:I:130:LEU:HD13	1:I:130:LEU:H	1.87	0.40
1:i:105:PRO:CG	1:i:173:GLN:HE21	2.35	0.40
1:Q:150:ALA:O	1:Q:152:LYS:HE3	2.22	0.40
1:1:151:GLY:HA3	1:o:104:VAL:HG13	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:148:LEU:O	1:Y:97:GLN:OE1[1_655]	2.04	0.16

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	100/157 (64%)	92 (92%)	7 (7%)	1 (1%)	12 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	112/157 (71%)	105 (94%)	7 (6%)	0	100	100
1	2	79/157 (50%)	74 (94%)	5 (6%)	0	100	100
1	3	94/157 (60%)	88 (94%)	6 (6%)	0	100	100
1	4	122/157 (78%)	107 (88%)	15 (12%)	0	100	100
1	5	123/157 (78%)	115 (94%)	7 (6%)	1 (1%)	16	50
1	A	96/157 (61%)	88 (92%)	7 (7%)	1 (1%)	12	45
1	C	121/157 (77%)	103 (85%)	18 (15%)	0	100	100
1	E	103/157 (66%)	98 (95%)	5 (5%)	0	100	100
1	G	123/157 (78%)	115 (94%)	8 (6%)	0	100	100
1	I	121/157 (77%)	110 (91%)	11 (9%)	0	100	100
1	K	108/157 (69%)	95 (88%)	12 (11%)	1 (1%)	14	48
1	M	118/157 (75%)	113 (96%)	5 (4%)	0	100	100
1	O	90/157 (57%)	84 (93%)	6 (7%)	0	100	100
1	Q	113/157 (72%)	105 (93%)	6 (5%)	2 (2%)	6	31
1	S	122/157 (78%)	119 (98%)	3 (2%)	0	100	100
1	U	89/157 (57%)	88 (99%)	1 (1%)	0	100	100
1	W	120/157 (76%)	116 (97%)	4 (3%)	0	100	100
1	Y	125/157 (80%)	120 (96%)	4 (3%)	1 (1%)	16	50
1	a	85/157 (54%)	85 (100%)	0	0	100	100
1	c	112/157 (71%)	105 (94%)	7 (6%)	0	100	100
1	e	122/157 (78%)	114 (93%)	7 (6%)	1 (1%)	16	50
1	g	121/157 (77%)	117 (97%)	4 (3%)	0	100	100
1	i	87/157 (55%)	77 (88%)	10 (12%)	0	100	100
1	k	93/157 (59%)	92 (99%)	1 (1%)	0	100	100
1	m	121/157 (77%)	110 (91%)	11 (9%)	0	100	100
1	o	43/157 (27%)	41 (95%)	2 (5%)	0	100	100
1	q	31/157 (20%)	29 (94%)	2 (6%)	0	100	100
1	s	90/157 (57%)	86 (96%)	4 (4%)	0	100	100
1	u	100/157 (64%)	93 (93%)	7 (7%)	0	100	100
1	w	35/157 (22%)	31 (89%)	4 (11%)	0	100	100
1	y	81/157 (52%)	79 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	6	9/15 (60%)	9 (100%)	0	0	100	100
2	7	9/15 (60%)	7 (78%)	2 (22%)	0	100	100
2	8	6/15 (40%)	6 (100%)	0	0	100	100
2	9	6/15 (40%)	5 (83%)	1 (17%)	0	100	100
2	B	8/15 (53%)	7 (88%)	1 (12%)	0	100	100
2	D	9/15 (60%)	8 (89%)	1 (11%)	0	100	100
2	F	9/15 (60%)	8 (89%)	0	1 (11%)	0	1
2	H	9/15 (60%)	7 (78%)	1 (11%)	1 (11%)	0	1
2	J	9/15 (60%)	8 (89%)	1 (11%)	0	100	100
2	L	9/15 (60%)	8 (89%)	1 (11%)	0	100	100
2	N	9/15 (60%)	9 (100%)	0	0	100	100
2	P	9/15 (60%)	8 (89%)	1 (11%)	0	100	100
2	R	9/15 (60%)	8 (89%)	1 (11%)	0	100	100
2	T	9/15 (60%)	7 (78%)	2 (22%)	0	100	100
2	V	8/15 (53%)	8 (100%)	0	0	100	100
2	X	10/15 (67%)	9 (90%)	1 (10%)	0	100	100
2	Z	9/15 (60%)	8 (89%)	1 (11%)	0	100	100
2	b	8/15 (53%)	8 (100%)	0	0	100	100
2	d	9/15 (60%)	7 (78%)	2 (22%)	0	100	100
2	f	9/15 (60%)	8 (89%)	1 (11%)	0	100	100
2	h	8/15 (53%)	8 (100%)	0	0	100	100
2	j	2/15 (13%)	2 (100%)	0	0	100	100
2	l	3/15 (20%)	3 (100%)	0	0	100	100
2	n	9/15 (60%)	8 (89%)	1 (11%)	0	100	100
2	p	3/15 (20%)	3 (100%)	0	0	100	100
2	t	4/15 (27%)	3 (75%)	1 (25%)	0	100	100
2	v	6/15 (40%)	6 (100%)	0	0	100	100
2	x	2/15 (13%)	1 (50%)	1 (50%)	0	100	100
2	z	3/15 (20%)	2 (67%)	1 (33%)	0	100	100
All	All	3412/5459 (62%)	3183 (93%)	219 (6%)	10 (0%)	36	70

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	151	GLY
1	K	107	GLU
1	5	116	LYS
1	Y	126	GLN
1	A	103	PHE
1	0	68	VAL
1	Q	98	ASP
2	H	793	PRO
1	e	84	GLY
2	F	793	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	94/132 (71%)	91 (97%)	3 (3%)	34	67
1	1	100/132 (76%)	97 (97%)	3 (3%)	36	69
1	2	79/132 (60%)	75 (95%)	4 (5%)	21	55
1	3	88/132 (67%)	84 (96%)	4 (4%)	24	59
1	4	110/132 (83%)	106 (96%)	4 (4%)	31	65
1	5	110/132 (83%)	101 (92%)	9 (8%)	10	37
1	A	92/132 (70%)	89 (97%)	3 (3%)	33	67
1	C	109/132 (83%)	102 (94%)	7 (6%)	16	48
1	E	96/132 (73%)	92 (96%)	4 (4%)	26	61
1	G	109/132 (83%)	103 (94%)	6 (6%)	19	53
1	I	107/132 (81%)	100 (94%)	7 (6%)	15	47
1	K	98/132 (74%)	89 (91%)	9 (9%)	8	33
1	M	107/132 (81%)	100 (94%)	7 (6%)	15	47
1	O	89/132 (67%)	85 (96%)	4 (4%)	24	59
1	Q	104/132 (79%)	100 (96%)	4 (4%)	29	63
1	S	108/132 (82%)	103 (95%)	5 (5%)	24	58
1	U	89/132 (67%)	83 (93%)	6 (7%)	15	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	111/132 (84%)	104 (94%)	7 (6%)	16	48
1	Y	111/132 (84%)	102 (92%)	9 (8%)	11	38
1	a	84/132 (64%)	78 (93%)	6 (7%)	13	43
1	c	102/132 (77%)	95 (93%)	7 (7%)	14	45
1	e	108/132 (82%)	101 (94%)	7 (6%)	15	47
1	g	109/132 (83%)	102 (94%)	7 (6%)	16	48
1	i	85/132 (64%)	75 (88%)	10 (12%)	5	22
1	k	91/132 (69%)	85 (93%)	6 (7%)	15	46
1	m	109/132 (83%)	100 (92%)	9 (8%)	10	37
1	o	55/132 (42%)	55 (100%)	0	100	100
1	q	41/132 (31%)	41 (100%)	0	100	100
1	s	89/132 (67%)	87 (98%)	2 (2%)	45	74
1	u	89/132 (67%)	84 (94%)	5 (6%)	19	52
1	w	43/132 (33%)	41 (95%)	2 (5%)	23	58
1	y	83/132 (63%)	76 (92%)	7 (8%)	10	37
2	6	10/13 (77%)	10 (100%)	0	100	100
2	7	10/13 (77%)	10 (100%)	0	100	100
2	8	7/13 (54%)	5 (71%)	2 (29%)	0	2
2	9	7/13 (54%)	7 (100%)	0	100	100
2	B	9/13 (69%)	9 (100%)	0	100	100
2	D	10/13 (77%)	10 (100%)	0	100	100
2	F	10/13 (77%)	10 (100%)	0	100	100
2	H	10/13 (77%)	10 (100%)	0	100	100
2	J	10/13 (77%)	10 (100%)	0	100	100
2	L	10/13 (77%)	10 (100%)	0	100	100
2	N	10/13 (77%)	8 (80%)	2 (20%)	1	7
2	P	10/13 (77%)	8 (80%)	2 (20%)	1	7
2	R	10/13 (77%)	9 (90%)	1 (10%)	7	29
2	T	10/13 (77%)	10 (100%)	0	100	100
2	V	9/13 (69%)	8 (89%)	1 (11%)	6	25
2	X	11/13 (85%)	11 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Z	10/13 (77%)	9 (90%)	1 (10%)	7	29
2	b	9/13 (69%)	9 (100%)	0	100	100
2	d	10/13 (77%)	10 (100%)	0	100	100
2	f	10/13 (77%)	9 (90%)	1 (10%)	7	29
2	h	9/13 (69%)	6 (67%)	3 (33%)	0	1
2	j	3/13 (23%)	3 (100%)	0	100	100
2	l	6/13 (46%)	6 (100%)	0	100	100
2	n	10/13 (77%)	10 (100%)	0	100	100
2	p	5/13 (38%)	4 (80%)	1 (20%)	1	7
2	r	2/13 (15%)	2 (100%)	0	100	100
2	t	7/13 (54%)	6 (86%)	1 (14%)	3	16
2	v	7/13 (54%)	6 (86%)	1 (14%)	3	16
2	x	3/13 (23%)	2 (67%)	1 (33%)	0	1
2	z	5/13 (38%)	5 (100%)	0	100	100
All	All	3248/4614 (70%)	3058 (94%)	190 (6%)	18	51

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	LEU
1	A	169	LEU
1	A	179	GLN
1	0	112	MSE
1	0	148	LEU
1	0	154	LEU
1	k	88	LEU
1	k	112	MSE
1	k	116	LYS
1	k	130	LEU
1	k	152	LYS
1	k	159	THR
1	m	107	GLU
1	m	112	MSE
1	m	130	LEU
1	m	133	HIS
1	m	145	ASP
1	m	152	LYS

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Mol	Chain	Res	Type
1	m	155	LEU
1	m	178	GLU
1	m	195	LEU
1	1	112	MSE
1	1	169	LEU
1	1	170	TRP
1	C	72	GLU
1	C	100	LYS
1	C	112	MSE
1	C	129	VAL
1	C	139	ILE
1	C	157	LEU
1	C	195	LEU
2	x	787	VAL
1	2	130	LEU
1	2	135	LEU
1	2	141	MSE
1	2	177	LEU
1	E	100	LYS
1	E	111	ILE
1	E	141	MSE
1	E	143	CYS
1	3	71	ILE
1	3	112	MSE
1	3	119	ILE
1	3	158	LYS
1	G	71	ILE
1	G	82	LEU
1	G	109	GLU
1	G	128	ASP
1	G	135	LEU
1	G	188	SER
2	8	784	LYS
2	8	788	THR
2	p	790	VAL
1	I	100	LYS
1	I	130	LEU
1	I	135	LEU
1	I	146	ASP
1	I	157	LEU
1	I	169	LEU
1	I	189	THR

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Mol	Chain	Res	Type
1	4	74	LEU
1	4	104	VAL
1	4	137	LEU
1	4	152	LYS
1	K	98	ASP
1	K	111	ILE
1	K	112	MSE
1	K	133	HIS
1	K	140	ARG
1	K	141	MSE
1	K	155	LEU
1	K	157	LEU
1	K	179	GLN
1	5	101	LEU
1	5	104	VAL
1	5	107	GLU
1	5	130	LEU
1	5	135	LEU
1	5	141	MSE
1	5	146	ASP
1	5	148	LEU
1	5	183	ILE
1	M	74	LEU
1	M	86	LEU
1	M	88	LEU
1	M	101	LEU
1	M	104	VAL
1	M	136	TYR
1	M	178	GLU
2	N	784	LYS
2	N	794	LYS
1	O	65	ILE
1	O	96	GLN
1	O	111	ILE
1	O	138	ILE
2	P	791	VAL
2	P	792	ASN
1	a	73	LYS
1	a	88	LEU
1	a	112	MSE
1	a	117	TYR
1	a	135	LEU

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Mol	Chain	Res	Type
1	a	152	LYS
1	s	88	LEU
1	s	112	MSE
2	t	784	LYS
1	u	107	GLU
1	u	112	MSE
1	u	131	HIS
1	u	145	ASP
1	u	155	LEU
2	v	791	VAL
1	c	92	ILE
1	c	94	VAL
1	c	107	GLU
1	c	112	MSE
1	c	145	ASP
1	c	155	LEU
1	c	165	GLU
1	e	91	TYR
1	e	93	ASP
1	e	97	GLN
1	e	107	GLU
1	e	112	MSE
1	e	145	ASP
1	e	155	LEU
2	f	794	LYS
1	g	86	LEU
1	g	88	LEU
1	g	104	VAL
1	g	107	GLU
1	g	130	LEU
1	g	136	TYR
1	g	178	GLU
2	h	787	VAL
2	h	788	THR
2	h	789	THR
1	i	82	LEU
1	i	88	LEU
1	i	89	ILE
1	i	112	MSE
1	i	155	LEU
1	i	157	LEU
1	i	160	THR

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Mol	Chain	Res	Type
1	i	172	TYR
1	i	173	GLN
1	i	179	GLN
1	Q	74	LEU
1	Q	88	LEU
1	Q	112	MSE
1	Q	166	GLU
2	R	792	ASN
1	S	86	LEU
1	S	88	LEU
1	S	104	VAL
1	S	136	TYR
1	S	178	GLU
1	U	74	LEU
1	U	86	LEU
1	U	88	LEU
1	U	104	VAL
1	U	136	TYR
1	U	178	GLU
2	V	789	THR
1	W	76	LEU
1	W	86	LEU
1	W	88	LEU
1	W	104	VAL
1	W	107	GLU
1	W	136	TYR
1	W	178	GLU
1	w	65	ILE
1	w	112	MSE
1	Y	73	LYS
1	Y	74	LEU
1	Y	83	GLU
1	Y	86	LEU
1	Y	88	LEU
1	Y	104	VAL
1	Y	130	LEU
1	Y	136	TYR
1	Y	178	GLU
1	y	86	LEU
1	y	88	LEU
1	y	90	ASN
1	y	107	GLU

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Mol	Chain	Res	Type
1	y	112	MSE
1	y	145	ASP
1	y	155	LEU
2	Z	784	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	133	HIS
1	0	90	ASN
1	0	179	GLN
1	k	173	GLN
1	m	179	GLN
1	1	173	GLN
1	C	90	ASN
1	C	97	GLN
1	C	173	GLN
1	C	179	GLN
1	E	173	GLN
1	3	173	GLN
1	3	175	ASN
2	B	792	ASN
2	r	792	ASN
1	I	126	GLN
1	I	181	GLN
1	4	173	GLN
1	4	179	GLN
2	J	792	ASN
1	K	179	GLN
1	5	90	ASN
1	5	133	HIS
1	O	179	GLN
1	s	131	HIS
1	u	164	ASN
1	u	179	GLN
1	c	97	GLN
1	c	179	GLN
1	e	179	GLN
1	i	131	HIS
1	i	173	GLN
1	S	96	GLN

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Mol	Chain	Res	Type
1	S	131	HIS
1	U	131	HIS
1	U	181	GLN
1	W	96	GLN
1	w	173	GLN
1	Y	96	GLN
1	Y	131	HIS
1	Y	164	ASN
1	Y	181	GLN
1	y	179	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	0	108/157 (68%)	-0.88	0	100 100	65, 77, 88, 97	0
1	1	116/157 (73%)	-0.87	0	100 100	66, 72, 83, 91	0
1	2	89/157 (56%)	-0.84	0	100 100	76, 85, 94, 97	0
1	3	102/157 (64%)	-0.71	0	100 100	75, 91, 105, 110	0
1	4	127/157 (80%)	-0.85	0	100 100	58, 76, 87, 90	0
1	5	126/157 (80%)	-0.88	0	100 100	55, 72, 82, 86	0
1	A	104/157 (66%)	-0.83	0	100 100	64, 77, 85, 90	0
1	C	125/157 (79%)	-0.86	0	100 100	46, 50, 56, 67	0
1	E	111/157 (70%)	-0.83	0	100 100	60, 73, 86, 95	0
1	G	125/157 (79%)	-0.92	0	100 100	58, 67, 79, 91	0
1	I	123/157 (78%)	-0.92	0	100 100	49, 57, 66, 77	0
1	K	114/157 (72%)	-0.89	0	100 100	55, 70, 82, 85	0
1	M	122/157 (77%)	-0.72	0	100 100	64, 78, 92, 105	0
1	O	100/157 (63%)	-0.74	0	100 100	73, 97, 116, 124	0
1	Q	120/157 (76%)	-0.81	0	100 100	72, 94, 106, 113	0
1	S	124/157 (78%)	-0.82	0	100 100	71, 87, 101, 110	0
1	U	99/157 (63%)	-0.52	0	100 100	82, 116, 134, 149	0
1	W	126/157 (80%)	-0.65	1 (0%)	82 64	67, 89, 106, 115	0
1	Y	127/157 (80%)	-0.81	0	100 100	67, 85, 107, 123	0
1	a	97/157 (61%)	-0.58	0	100 100	101, 119, 153, 158	0
1	c	118/157 (75%)	-0.50	0	100 100	91, 116, 149, 159	0
1	e	124/157 (78%)	-0.72	0	100 100	68, 92, 108, 116	0
1	g	125/157 (79%)	-0.64	0	100 100	87, 106, 120, 134	0
1	i	99/157 (63%)	-0.69	0	100 100	79, 105, 118, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	k	103/157 (65%)	-0.54	0	100	100	90, 110, 125, 131	0
1	m	125/157 (79%)	-0.75	0	100	100	75, 98, 110, 120	0
1	o	61/157 (38%)	-0.63	0	100	100	64, 112, 132, 147	0
1	q	45/157 (28%)	-0.62	0	100	100	73, 107, 121, 127	0
1	s	100/157 (63%)	-0.69	1 (1%)	79	59	89, 112, 129, 134	0
1	u	104/157 (66%)	-0.51	1 (0%)	79	59	88, 116, 139, 147	0
1	w	47/157 (29%)	-0.71	0	100	100	77, 107, 133, 139	0
1	y	91/157 (57%)	-0.47	0	100	100	106, 134, 155, 168	0
2	6	11/15 (73%)	-0.86	0	100	100	72, 77, 82, 90	0
2	7	11/15 (73%)	-0.99	0	100	100	66, 72, 75, 75	0
2	8	8/15 (53%)	-0.86	0	100	100	68, 73, 79, 80	0
2	9	8/15 (53%)	-0.94	0	100	100	64, 70, 78, 79	0
2	B	10/15 (66%)	-0.68	0	100	100	54, 69, 74, 75	0
2	D	11/15 (73%)	-0.98	0	100	100	36, 38, 64, 71	0
2	F	11/15 (73%)	-0.84	0	100	100	44, 65, 79, 80	0
2	H	11/15 (73%)	-0.98	0	100	100	46, 54, 63, 63	0
2	J	11/15 (73%)	-0.31	0	100	100	78, 83, 104, 112	0
2	L	11/15 (73%)	-1.05	0	100	100	59, 64, 70, 72	0
2	N	11/15 (73%)	-1.00	0	100	100	61, 66, 75, 80	0
2	P	11/15 (73%)	-0.99	0	100	100	45, 70, 90, 92	0
2	R	11/15 (73%)	-0.52	0	100	100	75, 85, 102, 104	0
2	T	11/15 (73%)	-0.91	0	100	100	80, 84, 87, 87	0
2	V	10/15 (66%)	-0.67	0	100	100	67, 71, 92, 93	0
2	X	12/15 (80%)	-0.71	0	100	100	64, 73, 80, 81	0
2	Z	11/15 (73%)	-0.69	0	100	100	87, 90, 92, 93	0
2	b	10/15 (66%)	-0.71	0	100	100	88, 100, 116, 117	0
2	d	11/15 (73%)	-0.76	0	100	100	65, 90, 99, 101	0
2	f	11/15 (73%)	-0.54	0	100	100	73, 78, 81, 83	0
2	h	10/15 (66%)	-0.79	0	100	100	78, 88, 93, 94	0
2	j	4/15 (26%)	-0.78	0	100	100	90, 92, 92, 95	0
2	l	7/15 (46%)	-0.87	0	100	100	72, 80, 99, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
2	n	11/15 (73%)	-0.70	0	100	100	89, 92, 94, 95	0
2	p	5/15 (33%)	-0.63	0	100	100	111, 117, 118, 121	0
2	r	2/15 (13%)	-1.32	0	100	100	76, 76, 76, 82	0
2	t	8/15 (53%)	-0.89	0	100	100	53, 57, 92, 94	0
2	v	8/15 (53%)	-0.40	0	100	100	80, 88, 104, 104	0
2	x	4/15 (26%)	-0.97	0	100	100	74, 78, 80, 83	0
2	z	5/15 (33%)	-0.99	0	100	100	99, 102, 108, 109	0
All	All	3703/5474 (67%)	-0.75	3 (0%)	92	86	36, 87, 129, 168	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	174	CYS	3.6
1	u	97	GLN	2.5
1	s	188	SER	2.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.